Qualitative and Quantitative Reasoning About Thermodynamics

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Abstract: One goal of qualitative physics is to capture the mental models of engineers and scientists. This paper shows how Qualitative Process theory can be used to express concepts of engineering thermodynamics. This encoding provides the means to integrate qualitative and quantitative knowledge for solving textbook thermodynamics problems. These ideas have been implemented in a program called `SCHISM`, which analyzes thermodynamic cycles, such as gas turbine plants and steam power plants. We describe its analysis of a sample textbook problem and discuss our plans for future work.

1 INTRODUCTION

A goal of qualitative physics is to capture the tacit knowledge engineers use to organize and control knowledge gained through formal training. The initial motivation for qualitative physics was to set up and guide the solution of textbook motion problems [6]. Since then, research has mainly focused on purely qualitative reasoning [2], and significant progress has been made. We believe the time is right to begin exploring the integration of qualitative and quantitative reasoning again. In particular, our long-range goal is to develop a system which can automatically perform engineering analyses of thermodynamic systems in a human-like way. This paper describes our first step towards that goal.

Studies of textbook problem solving have tended to focus on quantitative reasoning [1,4,14,15]. We begin instead with the view that qualitative models are the starting point for the accumulation and use of more sophisticated, quantitative models. This view is widely held in the mental models literature [11], and widely but less formally in the engineering community [16,17]. In problem-solving, the analysis begins by constructing a qualitative understanding of the situation. This initial understanding provides the framework for further analyses, such as deriving and solving sets of equations. Developing a correct qualitative understanding of the problem is essential to solving complex problems. Qualitative physics should provide the foundation for a more complete, formal account of human mental models, including how qualitative and quantitative knowledge interact.

This paper shows how Qualitative Process theory [8] can be used to encode fundamental concepts of engineering thermodynamics. This qualitative knowledge is used for problem solving in several ways. Qualitative simulation is used to verify that questions make sense by ensuring that the behavior mentioned can actually occur. The simulation also provides a framework for extracting equations. For example, heuristics for choosing appropriate control volumes are based on qualitative criteria. We have tested these ideas through implementation in a program called `SCHISM`, which solves textbook thermodynamics problems involving cycles.

The next section shows how a set of fundamental thermodynamic concepts can be encoded in QP theory. Section 3 describes how this encoding can be used as a basis for equation extraction and quantitative analysis. Section 4 describes `SCHISM`. Lastly, Section 5 demonstrates our ideas with an example of `SCHISM` analyzing the efficiency of a simple steam plant.

2 QP THEORY AND THERMODYNAMICS

Thermodynamics deals with transformations of energy from one form to another. The notion of process is central to thermodynamics, hence QP theory should be well-suited for representing it. Here we show how the following fundamental concepts of thermodynamics can be expressed in QP theory: *control volumes, closed cycles, equilibrium, steady state, phase changes, special processes,* and *point and path quantities.*

2.1 CONTROL VOLUMES

Every thermodynamic analysis starts by partitioning the universe into a *system* or *control volume* and its surroundings. A system is any macroscopic object or region of space selected for analysis. Systems are divided into three classes: *open*, *closed* and *isolated.* Open systems (such as the human body) exchange matter with their surroundings. Closed systems (e.g., the coolant in a refrigerator) allow energy but not matter to be exchanged with their surroundings. Isolated systems exchange neither mass nor energy with their surroundings.

Control volumes in a QP model correspond to individuals with the quantity `volume`, and contiguous collections of such individuals. The contained stuff ontology [12], used in our model, provides a natural partioning of an apparatus into macroscopic control volumes. "The coolant in the room coils of the refrigerator" is an example of a contained stuff. Our *Molecular Collection* (`MC`) ontology [5], which follows an infinitesimal piece of fluid through an apparatus, provides another useful control volume. An `MC` may be viewed as a closed control volume since its mass does not change. The `MC` control volume lets us describe properties of a fluid at a point in space.

In QP theory, open control volumes are easily identified as those which take part in some process that causes a mass transfer (such as `liquid-flow` or `boiling`). Closed control volumes are those which are not open but which participate in some work or heat transfer. Heat transfer and work transfer are indicated by participation in a `heat-flow` or `work-flow` process, respectively. A control volume is isolated if it does not participate in mass, work, or heat transfers.

2.2 CLOSED CYCLES

An important class of thermodynamic systems are *closed cycles.* In such systems, fluid continuously passes around a closed loop. Closed cycles are of great practical importance since they form the basis of heating, cooling and power generation systems. Indeed, whole books are written about the analysis of such systems [13]. Closed cycles are the first class of systems we have chosen for automated analysis by `SCHISM`.

The `MC` ontology provides a simple way to detect closed cycles, since a closed cycle directly corresponds to a cycle in the `MC` envisionment. Recognizing closed cycles allows `SCHISM` to select states of the envisionment that have the intended behavior as candidates for further analysis. (This also allows `SCHISM` to reject questions about impossible behaviors.)

2.3 PHASE CHANGES

Many engineering systems, such as refrigerators and steam plants, rely on phase changes to operate. These phase changes are modelled as processes in QP theory. `SCHISM` includes a model of boiling and of condensation. Unlike previous models, these processes include the thermal effects of mixing in the destination gas for boiling and the destination liquid for condensation.

2.4 EQUILIBRIUM

Equilibrium is the absence of certain processes acting. It is important enough to be explicitly represented, so we use views whose quantity conditions are the equality of driving forces. For example, the following view is active whenever two objects with a connecting heat path have the same temperature:

```
(defview (Thermal-Equilibrium ?src ?dst ?path)
    Individuals ((?src  :conditions (Quantity (Temperature ?src)))
                 (?dst  :conditions (Quantity (Temperature ?dst)))
                 (?path :conditions (heat-path ?path)
                                    (path-to ?path ?src ?dst)))
    Preconditions ((Heat-aligned ?path))
    QuantityConditions ((equal-to (A (temperature ?src))
                                  (A (temperature ?dst)))))
```

2.5 STEADY STATE

Another vital concept in thermodynamics is *steady state*. An apparatus is said to be in steady state when all point properties are constant with respect to time. This is the normal mode of operation for continuous flow processes. For example, when your kitchen refrigerator is running continuously, the temperature of the coolant at any point along the room coils is constant. Engineering analyses of thermodynamic cycles focus on steady state behavior.

In the QP model, a steady state system is indicated when all time derivatives of point properties are zero. When performing a steady-state analysis, these derivative constraints are added to QPE's scenario model so that only steady-state behaviors are envisioned[1]. If the envisionment is empty under this constraint, steady state behavior is impossible given the qualitative description of the system. Sometimes there is more than one steady state behavior (for example, the same apparatus could be used as a gas turbine power plant or an air cycle refrigerator, depending on driving conditions). If there is more than one steady-state behavior, teleology is used to select the appropriate state for further analysis.

2.6 SPECIAL PROCESSES

Quantitative analyses of closed systems are greatly simplified when processes drive parameters through particular trajectories in state space. Thermodynamic analyses often approximate real systems by assuming processes follow such trajectories. These approximations include:

- constant volume, or *isometric*
- constant pressure, or *isobaric*
- constant temperature, or *isothermal*
- *adiabatic*, ie., no heat flow crosses the system boundary.

For example, boiling is generally approximated as an isothermal process. These exact distinctions can be drawn about the processes in the QP model. Isometric, isobaric, and isothermal processes can be recognized by noting the sign of the appropriate derivative. Adiabatic processes can be recognized by the absence of active heat flow processes between the system and its environment.

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[1] QPE is an envisioner for QP theory. For details see [9].

2.7 POINT AND PATH QUANTITIES

Thermodynamics distinguishes between *path-independent* and *path-dependent* parameters. Path-independent parameters, also known as *point properties* or *state functions* of a substance, include temperature, pressure and volume. They can be determined directly from the current values of other parameters. For example, fixing the pressure and volume of a gas uniquely determines its temperature. Path-dependent parameters (often called "absolute flows") are integrals of flow rates. Examples include work, mass flow, and heat flow. Computing path-dependent parameters requires histories; For example, the amount of work required to compress a gas from state S_1 to S_2 depends on how the compression is done. Compression may occur isothermally, adiabatically or along some arbitrary path.

Path-independent parameters are always explicit properties of individuals in the QP domain model. Flow rates are always explicit properties of processes in the QP domain model (e.g., `mass-flow-rate`, `heat-flow-rate`). Since `SCHISM` currently focuses on steady-state problems, we have not yet implemented path-dependent properties.

3 EXTRACTING EQUATIONS

The interaction of qualitative and quantitative reasoning used in classical thermodynamic analyses is common in the interdisciplinary field called *mathematical modelling.* Experts in the field regard math modelling as something of an art [16]:

> "It should now be apparent that an understanding of the scientific motivation of the problem and the ability to use heuristic reasoning, as *well* as manipulative skill, are essential to the practice of applied mathematics."

We claim mathematical modelling of physical phenomena begins with a qualitative model. Equations are extracted from the qualitative model until a tractable *closed* set is obtained. A closed set of equations is a set of n independent equations that contains n or fewer unknowns. If the equations are intractable, simplifying assumptions may be added to the qualitative model. An example of a simplifying assumption in thermodynamics is *adiabaticity* of a process.

The equations which can be extracted from a model can be divided into three classes. *Domain principles P* include fundamental laws and empirical correlations such as conservation of mass and equations of state. *Domain definitions D* introduce new quantities by defining them in terms of existing ones. An example is the efficiency of a system behaving as a heat engine, which is defined to be the rate of work flowing into the system divided by the rate of work flowing out. *Qualitative identities I* are equations that are derivable directly from relations in the qualitative model. For example, the qualitative model of a dammed river at steady state will include the relation that the flow rate of water into the lake equals the flow rate of water out.

In thermodynamics, extracting an equation from a qualitative state consists of two steps: (1) choosing a control volume v from the set of possible control volumes V, and (2) applying to that control volume a domain principle $p \epsilon P$, domain definition $d \epsilon D$, or qualitative identity $i \epsilon I$.

The number of possible equations that can be extracted from a given qualitative state is thus $| V \times (P \cup D \cup I) |$. This number can be enormous. In thermodynamics, choosing the right control volumes is crucial to the efficient search of the equation space. For example, instantiating the ideal gas law for a contained gas about which nothing is known introduces four new variables: the temperature, pressure, volume and mass of the contained gas. This moves us further from the goal of a closed set of equations.

While the qualitative model provides all possible control volumes, the subset which is actually useful tends to be small. We have developed a heuristic technique for ordering the possibilities. The control volumes are divided into lexicographically ordered classes using five essentially qualitative criteria:

1. *Boundary Conditions:* Prefer systems which border goal flow rate quantities.
2. *Geometry:* Prefer systems whose boundaries are crossed by fewer flows.
3. *Number of Knowns:* Prefer systems containing many known quantities.
4. *Boundary Homogeneity:* Prefer systems where only a single type of flow (e.g., only heat flow) crosses its boundary.
5. *Internal Complexity:* Prefer smaller, simpler control volumes.

In the example below, these heuristics enabled `SCHISM` to narrow its search to a small fraction of the total equation space.

4 HOW SCHISM WORKS

`SCHISM` is an approximately 7000 line lisp program consisting of three major parts that perform: (1) qualitative teleology analysis of program input, (2) equation space searching, and (3) symbolic math manipulations. It takes four inputs: (*i*) the intended function of the system, (*ii*) an envisionment of the system (generated by `QPE`), (*iii*) a set of quantitative facts and measurements of the system, and (*iv*) a goal quantity.

`SCHISM` begins an analysis by verifying that the apparatus behaves as intended. It does this by examining `QPE`'s envisionment. Currently, `SCHISM` recognizes two classes of thermodynamic systems, heat-engines and heat-pumps. If the expected behavior is that of a heat-engine, `SCHISM` checks that some state in the envisionment satisfies the following three criteria: (1) it contains a closed `MC` cycle, (2) it has a net flow of work *out* of the system, and (3) it transfers heat from a hotter place to a colder place. Each of these properties can be determined directly by inspecting the situation. This increases `SCHISM`'s robustness by allowing it to detect a class of nonsense questions.

`SCHISM` organizes its search through the equation space as an AND/OR tree[2] with the root goal node being to show that the goal quantity is known. To solve for the goal quantity, equations are extracted that contain the sought quantity. Closing these equations become the subgoals of the root. The unknown quantities in these subgoals are then sought at the next level of the tree, and so forth. During the search, `SCHISM` might choose to focus on a new control volume for each sought quantity, using the heuristics described earlier.

Once a closed set of equations containing the sought quantity is found, the equation space search halts. The final expression for the goal quantity is found by solving the set of equations via substitution. `SCHISM`'s symbolic math package includes a canonical rational function manipulator to perform simplification of most mathematical expressions. The *isolation, collection* and *attraction* methods of Bundy [3] are used for extracting variables from equations.

5 AN EXAMPLE

The following example is taken from [13]. In the text, Haywood introduces the steam plant shown in figure 5 by describing its parts, structure and qualitative behavior. The steam plant consists of

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[2] We use an extension of the `AO-SOLVE` system described in [10].

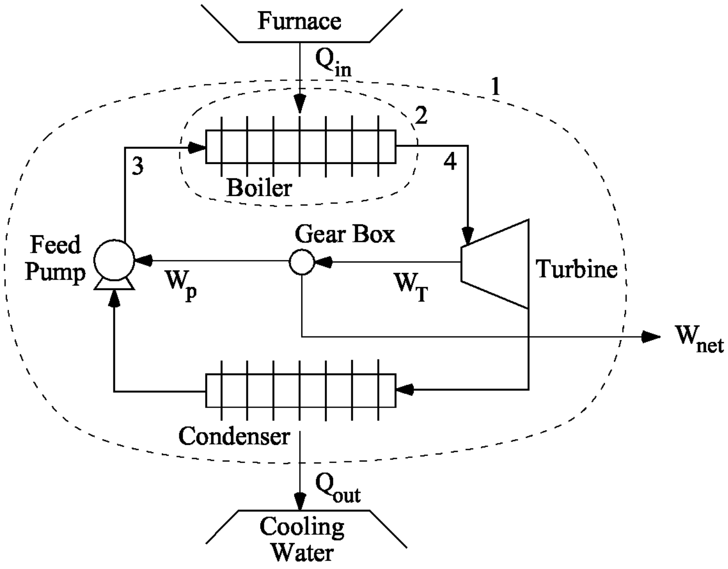

Figure 1: A Steam Plant

a turbine, condenser, feed pump, boiler, high temperature furnace, low temperature cooling water, and a gear box for splitting work output. Water enters the boiler at a low temperature and leaves as high-pressure steam. In the boiler, the fluid remains at approximately constant pressure while heat flows to it from the furnace. The steam flows through the turbine, dropping in pressure and temperature while producing work. The low temperature steam is then condensed at very nearly constant pressure while heat is transfered to the cooling water. The condensate is then pumped from the condenser into the boiler and the cycle repeats.

The problem statement is:

> **1.1.** In a test of a cyclic steam power plant, the measured rate of steam supply was 7.1 kg/s when the net rate of work output was 5000 kW. The feed water was supplied to the boiler at a temperature of 38°C, and the superheated steam leaving the boiler was at 1.4 MN/m^2 and 300°C. Calculate the thermal efficiency of the cycle.

From a `QPE` envisionment, `SCHISM` locates a contiguous set of control volumes (labelled 1 in figure 5) whose combined behavior does indeed match that of a heat engine. Since the goal quantity refers to a heat engine, this is the initial system choice from which equations are extracted.

A commonly used heuristic in the analysis of thermodynamic flow processes is *plunking* (as in [7]) of a system's mass flow rate. A plunked quantity is permitted to appear as a constant in the final solution. The plunking of a system's mass flow rate is equivalent to basing its analysis on the assumption of a unit mass flow rate. In this example, `SCHISM` infers that the closed cycle has a mass flow rate of 7.1 kg/s since that is the given flow rate of steam entering the turbine. Because the mass flow rate of the heat engine is known, `SCHISM` elects not to use the plunking heuristic.

`SCHISM` next initiates a search through the equation space. In our example, the control volume heuristic guides `SCHISM` to consider seven systems out of a possible 64. Two of the seven systems prove useful for extracting a set of closed equations.

(1) $\rho_1 = \sum_1 Q_{in} / \sum_1 W_{out}$

(2) $\sum_1 W_{out} = W_{net}$

(3) $W_{net} = 5000$

(4) $\sum_1 Q_{in} = Q_{in}$

(5) $\sum_2 nH + \sum_2 Q + \sum_2 W = 0$

(6) $\sum_2 Q = \sum_2 Q_{in} - \sum_2 Q_{out}$

(7) $\sum_2 Q_{in} = Q_{in}$

(8) $\sum_2 Q_{out} = 0$

(9) $\sum_2 W = \sum_2 W_{in} - \sum_2 W_{out}$

(10) $\sum_2 nH = \sum_2 (nH)_{in} - \sum_2 (nH)_{out}$

(11) $\sum_2 W_{in} = 0$

(12) $\sum_2 W_{out} = 0$

(13) $\sum_2 (nH)_{in} = n_3 H_3$

(14) $\sum_2 (nH)_{out} = n_4 H_4$

(15) $H_3 = \mathit{Table}(H, \mathit{water}, \mathit{liquid}, T_3)$

(16) $H_4 = \mathit{Table}(H, \mathit{water}, \mathit{gas}, T_4, P_4)$

(17) $n_3 = n_1$

(18) $n_4 = 7.1$

(19) $n_1 = n_4$

(20) $T_3 = 38$

(21) $T_4 = 300$

(22) $P_4 = 1.4$

(23) $\mathit{Table}(H, \mathit{water}, \mathit{liquid}, 38) = 159$

(24) $\mathit{Table}(H, \mathit{water}, \mathit{gas}, 300, 1.4) = 3041$

Notation: Thermodynamic symbols are defined below. Subscripts and summation indices refer to the control volumes and locations shown in figure 5. For example, $\sum_2 Q$ denotes the sum of the heat flow rates into and out of control volume 2 (the boiler). We use $\mathit{Table}(H, \mathit{water}, \mathit{gas}, T_4, P_4)$ to denote the tabulated intensive (ie., per unit mass) enthalpy value of water vapor at location 4.

Q = heat flow rate
W = work rate
n = mass flow rate
H = intensive enthalpy
T = temperature
P = pressure
ρ = efficiency

Figure 2: Steam plant equations generated by `SCHISM`

`SCHISM` spawns a total of 56 equations, 24 of which form a closed set (see Figure 5). Substitution of equations is then performed on the closed set to produce a final expression for the sought quantity: 0.244 (i.e., 24.4%) which is the correct answer.

6 DISCUSSION

We have shown how the language of QP theory is well suited for representing qualitative knowledge in the domain of engineering thermodynamics, and can serve as a framework for organizing other kinds of knowledge. The qualitative model provides four essential functions: (1) recognition/verification of the system's intended behavior, (2) establishing the set of possible control volumes, (3) heuristic guiding of the selection of control volumes in equation extraction (4) establishing the set of qualitative identities which contribute equations to the closed set.

While we do not view `SCHISM` as a cognitive simulation per se, we believe that our model for how qualitative and quantitative knowledge interact can provide a richer framework for explaining psychological data. For example, "keywords in the [problem] statement" have been conjectured as the basis for ignoring variables or setting their values to zero [1], which in `SCHISM` falls out through qualitative analysis. Further psychological studies might reveal a novice-expert shift, with novices using surface features and experts relying on a generative qualitative analysis [4].

At present `SCHISM` has been successfully tested on three examples, all from Chapter One of [13]. Our plan is to continue working through the textbook, seeing how much of it we can master by augmenting the set of equations and domain model as necessary. An interesting question we hope to answer is how large a role each kind of knowledge plays in mastering these problems. For example, we currently suspect that the number of specialized equation-solving techniques will continue to grow with the number of examples, while the qualitative model will stabilize more quickly. As we extend the range of problems `SCHISM` can solve, we hope to compare its performance with human subjects.

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